Predictive Science Academic Alliance Program (PSAAP)

The slides that follow were presented at the PSAAP Bidder's Meeting May 16-17, 2006 and represent the ASC Trilab authors and interests as presented in the associated White Paper for this subject area.

Nuclear Theory & ASC interests

Mark Chadwick, Bob Little
(presented by Gerry Hale)
Los Alamos National Laboratory
+ input from LANL theorists (Carlson, Moller, Kawano, Hayes, Hale)
+ input from Livermore theorists (Ormand, Navratil, Younes, Escher)

Focus areas:

- **Ab-initio predictions of light nucleus reactions**
- **Fission predictions**
- **Radiative neutron capture**

Application areas:

- **Astrophysical nucleosynthesis**
- **Advanced reactors & fuel cycles & transmutation**

Common theme:

a) predictive capability for unmeasured neutron cross sections
b) Use of high performance computing

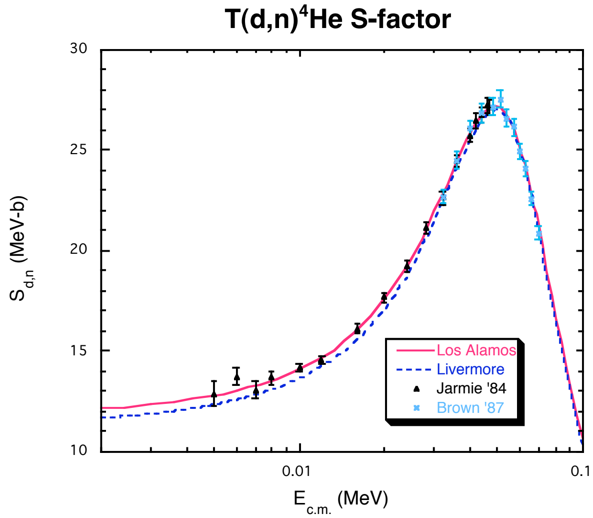
Light nucleus reactions

- Take advantage of some exciting theory advances in recent years, for using ab-initio methods to predict nuclear structure & reactions
    - reaction capability less advanced than structure & needs work
    - HPC advances open up new possibilities

- Various methods could be pursued:
    - Ab-initio shell model
    - Greens function Monte Carlo
    - etc.

- Some important needs
    - start with A=5 as test case (d+t). Resolve issues at low and high energies
    - A=7 system, for astrophysical needs
    - A=8 system, for astrophysics. Also, n+7Be (largely unmeasured)
    - A=9-16, relevant for NIF, astrophysics, etc. Large computers needed

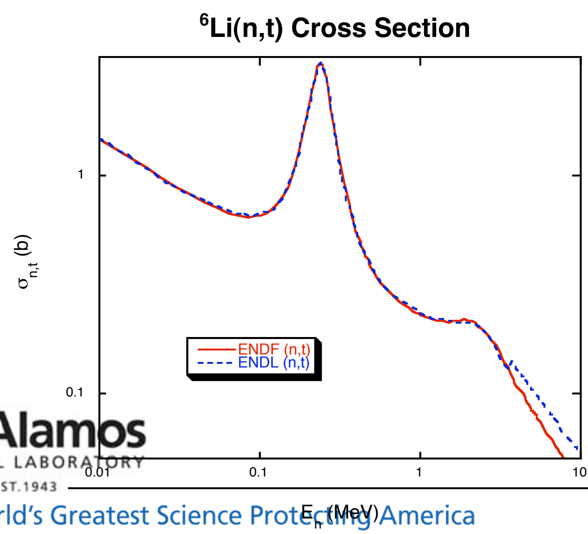
Differences for Important TN Reactions



— multi-level, multi-reaction analysis of data in ^{5}He system for $E \leq$ 6 MeV

--- single-level fit to ^{3}H(d,n) cross section data for $E \leq$ 0.12 MeV

Difference at low energies is ~ 4%.



Evaluated cross sections below and over the 240-keV resonance are similar.

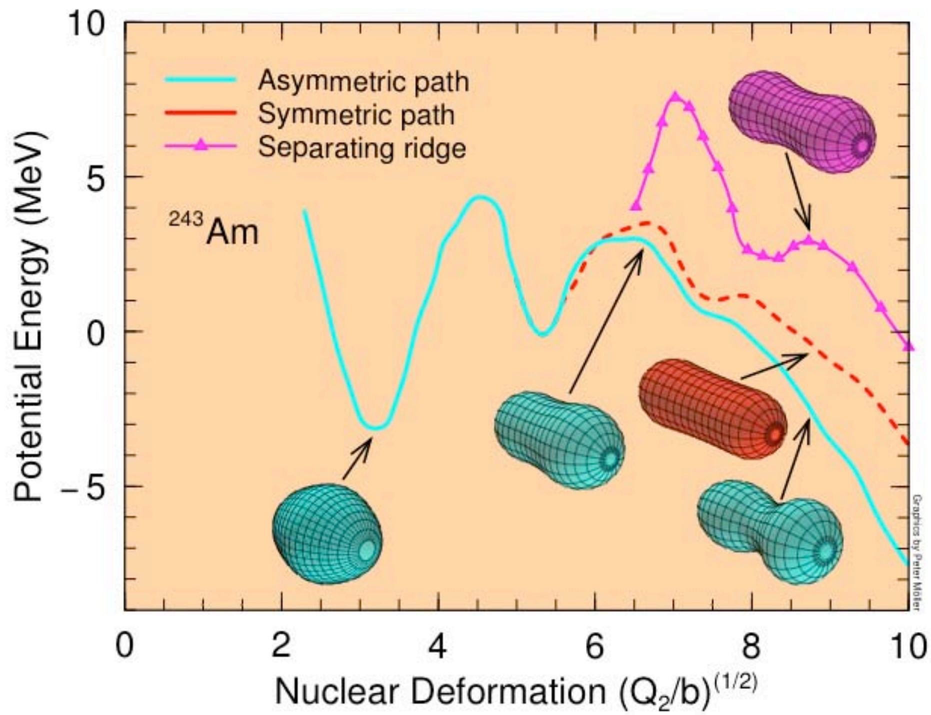
Differences become very large (> 40 %) above about 3.5 MeV.

Fission Physics: Synergy with Astrophysics & Advanced Reactor Needs

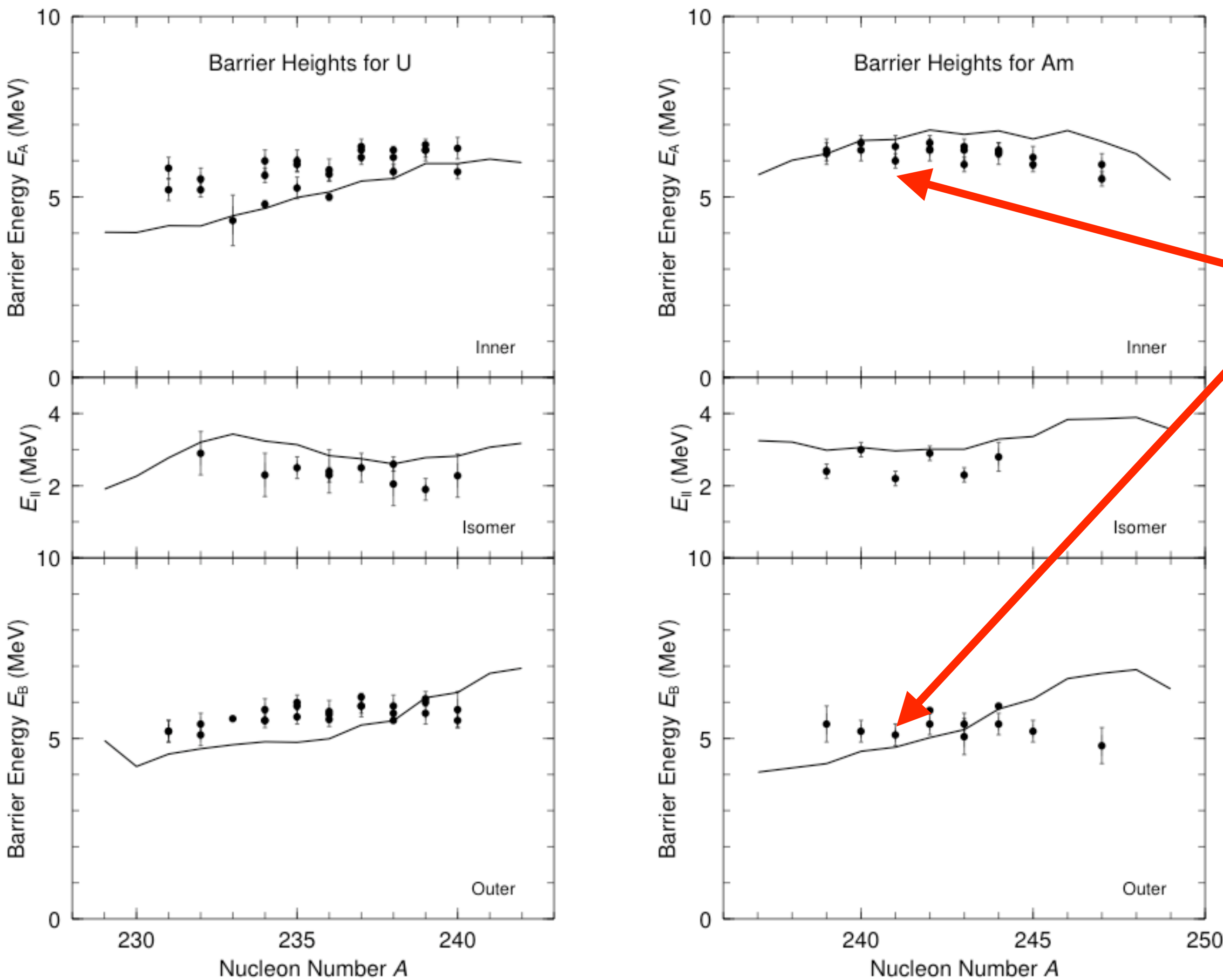
- Fission cross section modeling today uses both theory and **phenomenology**

- Need a predictive capability for:
  - -Off stability predictions (*e.g.* 237U, 240Am, …)
  - - post-scission physics (prompt gammas, neutrons, fragments, energy splits)

- Are there credible advances in theory that could lead to real predictive capability?
  - - the challenge is that the fission cross section depends so sensitively on barrier heights



New Advances in Fission Modeling. But still need improved predictions



Exp. data are not direct, but inferred.

241Am CN data from LANL transfer surrogate experiments (Wilhelmy, Britt, Gavron, et al.)

Axial asymmetry may reduce the calculated heights here.

(Fragments are axially asymmetric in shape).

Radiative Capture Predictions: Synergy with Astrophyics s,r-process, and with Reactor & Fuel Cycle Applications

• Capture cross section modeling today uses both theory and **phenomenology**

• Need a predictive capability for:
- -Stable and off stability nuclide predictions
- - Exp data often discrepant; rarely known to better than 20%, often factors 2-5
- - 0.5-1 MeV, very little data

• Are there credible advances in theory that could lead to real predictive capability?

The 0.5-1 MeV region is largely unmeasured.